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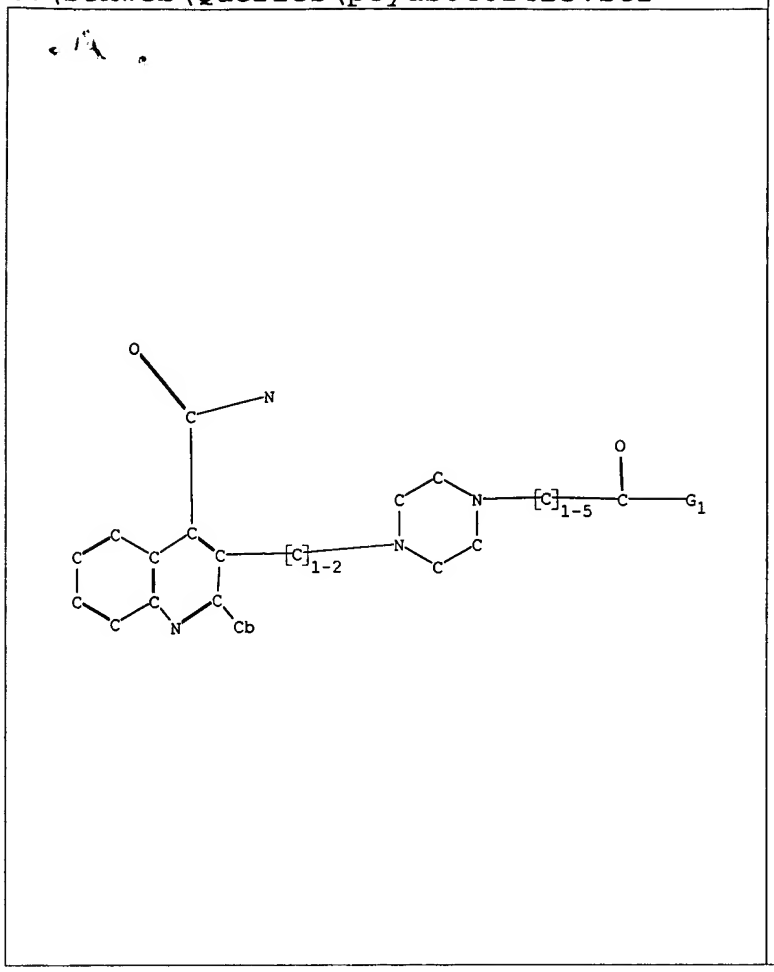

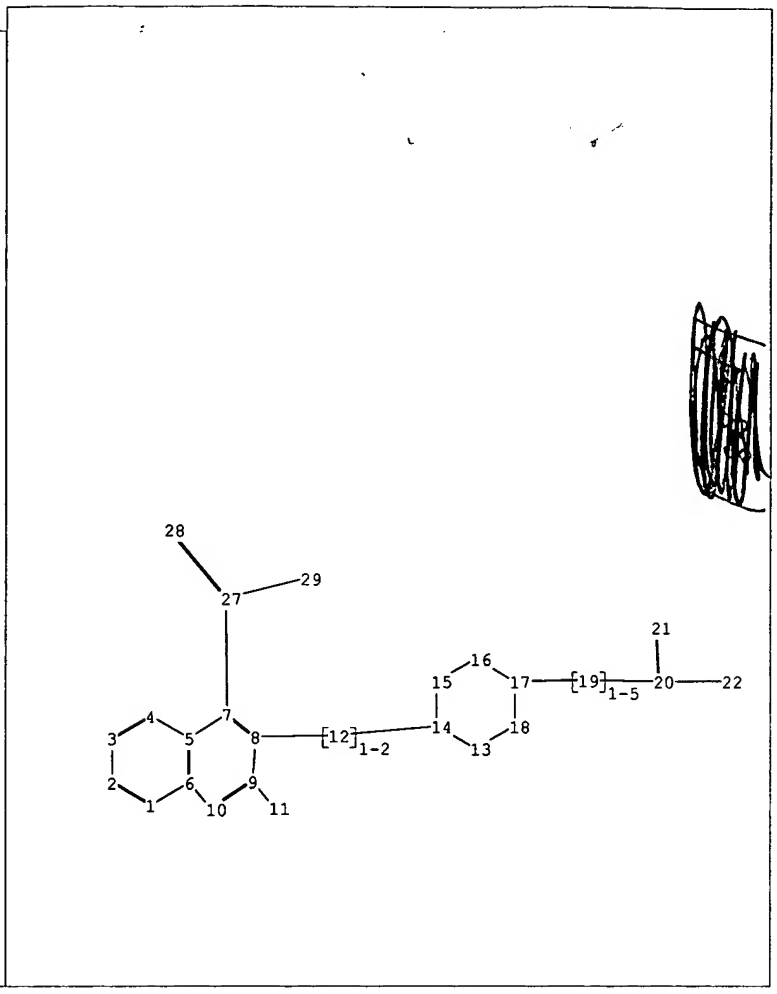

chain nodes :
11 12 19 20 21 22 27 28 29
ring nodes :
1 2 3 4 5 6 7 8 9 10 13 14 15 16 17 18
chain bonds :
7-27 8-12 9-11 12-14 17-19 19-20 20-21 20-22 27-28 27-29
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 13-14 13-18
14-15 15-16 16-17 17-18
exact/norm bonds :
12-14 13-14 13-18 14-15 15-16 16-17 17-18 17-19 20-21 20-22
27-28 27-29
exact bonds :
7-27 8-12 9-11 19-20
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10
isolated ring systems :
containing 1 :

G1:O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
18:Atom 19:CLASS 20:CLASS 21:CLASS 22:CLASS 27:CLASS 28:CLASS
29:CLASS
Generic attributes :

11:

Saturation	: Unsaturated
Number of Carbon Atoms	: less than 7
Type of Ring System	: Monocyclic

```
* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1           Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2           "Ask CAS" for self-help around the clock
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                   resulting in a closer connection to BABS
 NEWS  4  AUG 02   IFIPAT/IFIUDB/IFICDB reloaded with new search and display
                   fields
 NEWS  5  AUG 02   CAplus and CA patent records enhanced with European and Japan
                   Patent Office Classifications
 NEWS  6  AUG 02   The Analysis Edition of STN Express with Discover!
                   (Version 7.01 for Windows) now available
 NEWS  7  AUG 27   BIOCOMMERCE: Changes and enhancements to content coverage
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                   status data from INPADOC
 NEWS  9  SEP 01   INPADOC: New family current-awareness alert (SDI) available
 NEWS 10  SEP 01   New pricing for the Save Answers for SciFinder Wizard within
                   STN Express with Discover!
 NEWS 11  SEP 01   New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
 NEWS 12  SEP 27   STANDARDS will no longer be available on STN
 NEWS 13  SEP 27   SWETSCAN will no longer be available on STN

 NEWS EXPRESS  JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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FILE 'HOME' ENTERED AT 22:06:05 ON 27 OCT 2004

=> file reg
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                 0.21       0.21

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STRUCTURE FILE UPDATES:   26 OCT 2004  HIGHEST RN 769912-90-5
DICTIONARY FILE UPDATES:  26 OCT 2004  HIGHEST RN 769912-90-5
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TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L1      STRUCTURE UPLOADED

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SAMPLE SEARCH INITIATED 22:14:52 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      1 TO ITERATE

100.0% PROCESSED       1 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:             1 TO       80
PROJECTED ANSWERS:                0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 sss full
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FULL SCREEN SEARCH COMPLETED -     72 TO ITERATE

100.0% PROCESSED      72 ITERATIONS                               27 ANSWERS
SEARCH TIME: 00.00.01

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=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
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FILE 'CAPLUS' ENTERED AT 22:15:12 ON 27 OCT 2004
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FILE COVERS 1907 - 27 Oct 2004  VOL 141 ISS 18
FILE LAST UPDATED: 26 Oct 2004  (20041026/ED)
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This file contains CAS Registry Numbers for easy and accurate substance identification.

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L4 4 L3

=> d l4 1-4 bib abs hitstr

L4 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
Full Text
AN 2004:648346 CAPLUS
DN 141:190804
TI Preparation of quinoline derivatives as NK-2 and NK-3 receptor antagonists
IN Kerns, Jeffrey; Jin, Qi; Yan, Hongxing; Wan, Zehong
PA Smithkline Beecham Corporation, USA
SO PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004066951	A2	20040812	WO 2004-US2425	20040129

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PRAI US 2003-443598P P 20030130
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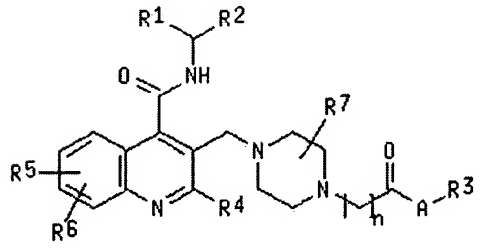


I

AB The title compds. [I; R1 = H, (un)substituted alkyl; R2 = (un)substituted aryl, cycloalkyl, heterocyclyl; R3 = H, (un)substituted alkyl, cycloalkyl, aryl, heterocyclyl; A = NR8, O (R8 = H, (un)substituted alkyl); R4 = (un)substituted Ph; R5 = H, alkyl, alkenyl, aryl, etc.; or R5 represents a bridging moiety which is arranged to bridge two adjacent ring atoms, wherein the bridging moiety comprises alkylene or dioxyalkylene; R6 = H, halo; R7 = oxo; n = 1-4] which are NK2 and NK3 receptor antagonists and are useful in the treatment of respiratory diseases, were prepd. Thus, treating 2-(3,5-difluorophenyl)-6-fluoro-3-(3-oxopiperazin-1-ylmethyl)-quinoline-4-carboxylic acid [(S)-1-cyclohexylethyl]amide with Et iodoacetate in the presence of NaH in DMSO followed purifn. via reverse

phase HPLC, and amidating the resulting acetic acid deriv. with 1-methylpiperazine afforded 2-(3,5-difluorophenyl)-6-fluoro-3-{4-[2-(4-methylpiperazin-1-yl)-2-oxoethyl]-3-oxopiperazin-1-ylmethyl}-quinoline-4-carboxylic acid [(S)-1-cyclohexylethyl]amide. The most potent compds. I show IC50 in the range 10-1000 nM against NK-3 receptor binding, and IC50 in the range 1-1000 nM against NK-2 receptor binding. The pharmaceutical compn. comprising the compd. I is claimed.

IT **736989-75-6P 736989-76-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

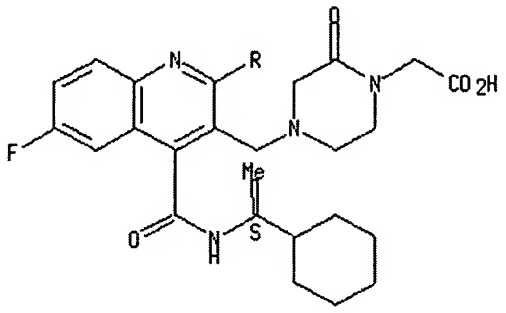
(prepn. of quinoline derivs. as NK-2 and NK-3 receptor antagonists for treating respiratory diseases)

RN 736989-75-6 CAPLUS

CN 1-Piperazineacetic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-2-(3,5-difluorophenyl)-6-fluoro-3-quinolinyl]methyl]-2-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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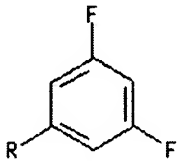
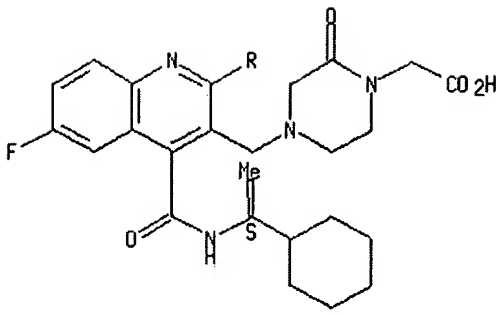
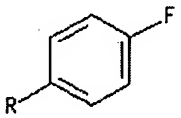


RN 736989-76-7 CAPLUS

CN 1-Piperazineacetic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-6-fluoro-2-(4-fluorophenyl)-3-quinolinyl]methyl]-2-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





L4 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
Full Text
AN 2002:428893 CAPLUS
DN 137:20387
TI Preparation of 3-(piperazinylalkyl)-4-quinolinecarboxamides as NK-3 and NK-2 antagonists for treatment of respiratory diseases and CNS disorders
IN Farina, Carlo; Gagliardi, Stefania; Giardina, Giuseppe; Grugni, Mario; Nadler, Guy Marguerite Marie Gerard; Martinelli, Marisa
PA Glaxosmithkline S.P.A., Italy; Laboratoire Glaxosmithkline S.A.S.
SO PCT Int. Appl., 119 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

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PI	WO 2002044165	A1	20020606	WO 2001-EP13833	20011126
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2002026356	A5	20020611	AU 2002-26356	20011126
	EP 1351953	A1	20031015	EP 2001-995670	20011126
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
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	US 2004097518	A1	20040520	US 2003-432925	20031124
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OS MARPAT 137:20387
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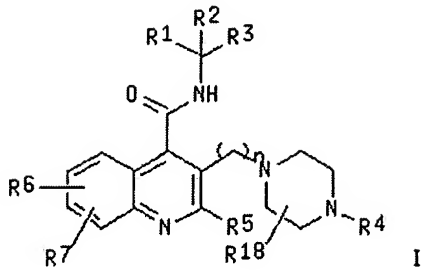

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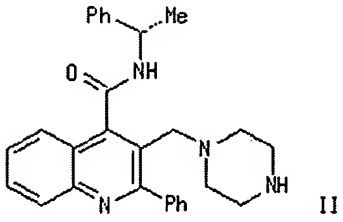


II

AB Title compds. I [wherein R1 = H or alkyl; R2 = (un)substituted (hetero)aryl or cycloalkyl; R3 = H, alkyl, or cycloalkyl(alkyl) (un)substituted by 1 or more fluorines; R4 = H or R8R9; R5 = branched or linear alkyl, cycloalkyl(alkyl), aryl, or single or fused-ring arom. (un)substituted heterocyclic group; R6 = H, or 1-3 of alkyl, alkenyl, aryl, alkoxy, OH, halo, NO2, cyano, CO2H, alkylcarboxy(alkyl), haloalkyl, NH2, or (di)(alkyl)amino; or R6 = a bridging alkyl or dioxyalkylene; R7 = H or halo; R8 = (un)substituted alkyl or alkenyl; R9 = S(O2)R10, S(O2)OR10, ONO, CO2R10, CONR11R12, or CN; R10 = H, (cyclo)alkyl, or aryl; R11 and R12 = independently H or alkyl; R18 = H or up to 3 oxo groups; any of R2, R5, R8, R10, R11, or R12 may be (un)substituted 1 or more times by halo, OH, NH2, cyano, NO2, CO2H, or oxo; n = 1-6; with 26 compds. excluded; and their pharmaceutically acceptable salts or hydrates] were prepd. I are a novel class of potent non-peptide neurokinin-3 (NK-3) antagonists, some of which fall within the generic scope of WO 00/31037. I are far more stable metabolically and show improved oral bioavailability compared to the known peptidic NK-3 receptor antagonists (no data). In addn., I have good NK-2 antagonist activity and are considered to be of potential use in the prevention and treatment of a wide variety of clin. conditions which are characterized by over-stimulation of tachykinin receptors, in particular NK-3 and NK-2. Forty-eight specific (S)-isomeric compds. I were prepd. For instance, 4-carboxy-3-methyl-2-phenylquinoline was subjected to the sequence of (1) Me esterification; (2) α-bromination; (3) amination of the bromide with piperazine-1-carboxylic acid tert-Bu ester; (4) ester hydrolysis (95%); and (5) amidation with (S)-1-phenylethylamine to give the title compd. II. In binding assays using human NK-2 receptors and guinea pig and human NK-3 receptors, the most potent I exhibited IC50 values ranging from 0.5 nM to 1000 nM and from 0.1 nM to 1000 nM, resp.

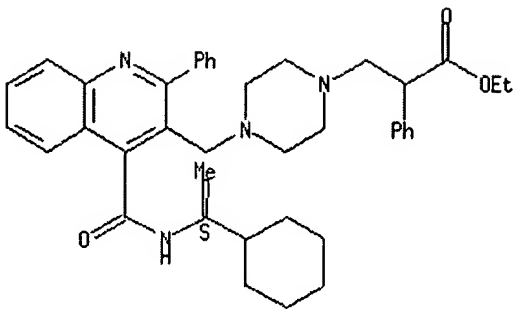
IT **433962-06-2P**

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(NT-2 and NT-3 receptor antagonist; prepn. of piperazinylalkyl quinolinecarboxamides as NK-3 and NK-2 antagonists for treatment of respiratory diseases and CNS disorders)

RN 433962-06-2 CAPLUS

CN 1-Piperazinepropanoic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-2-phenyl-3-quinolinyl]methyl]-α-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

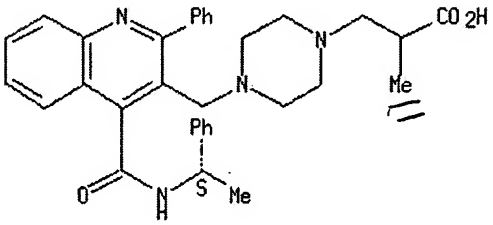
Absolute stereochemistry.



IT **433961-92-3P 433961-97-8P 433962-00-6P**
433962-02-8P 433962-04-0P 433962-11-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(NT-2 and NT-3 receptor antagonist; prepn. of piperazinylalkyl quinolinecarboxamides as NK-3 and NK-2 antagonists for treatment of respiratory diseases and CNS disorders)

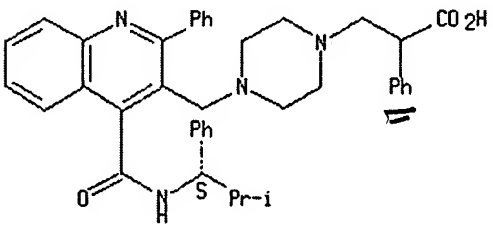
RN 433961-92-3 CAPLUS
CN 1-Piperazinepropanoic acid, α-methyl-4-[[2-phenyl-4-[[[(1S)-1-phenylethyl]amino]carbonyl]-3-quinolinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 433961-97-8 CAPLUS
CN 1-Piperazinepropanoic acid, 4-[[4-[[[(1S)-2-methyl-1-phenylpropyl]amino]carbonyl]-2-phenyl-3-quinolinyl]methyl]-α-phenyl- (9CI) (CA INDEX NAME)

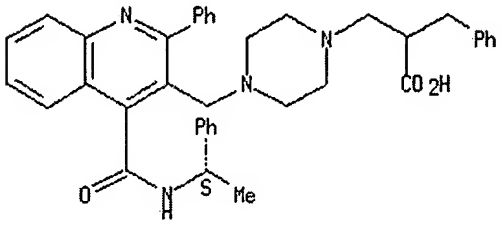
Absolute stereochemistry.



RN 433962-00-6 CAPLUS
CN 1-Piperazinepropanoic acid, α-(phenylmethyl)-4-[[2-phenyl-4-[[[(1S)-

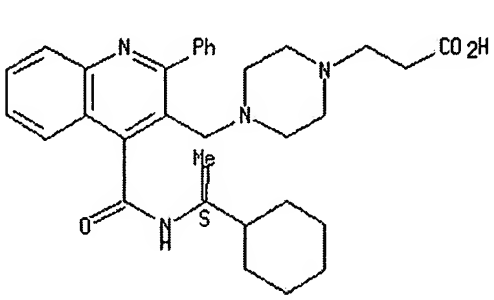
1-phenylethyl]amino]carbonyl]-3-quinolinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



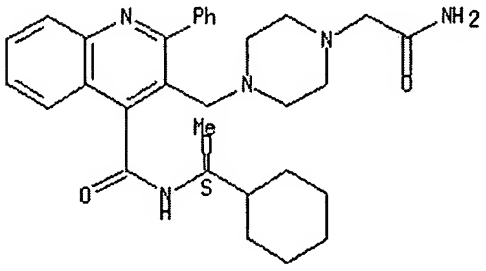
RN 433962-02-8 CAPLUS
CN 1-Piperazinepropanoic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-2-phenyl-3-quinolinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



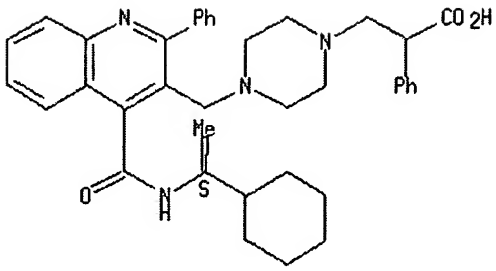
RN 433962-04-0 CAPLUS
CN 4-Quinolinecarboxamide, 3-[[4-(2-amino-2-oxoethyl)-1-piperazinyl]methyl]-N-[(1S)-1-cyclohexylethyl]-2-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 433962-11-9 CAPLUS
CN 1-Piperazinepropanoic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-2-phenyl-3-quinolinyl]methyl]-α-phenyl- (9CI) (CA INDEX NAME)

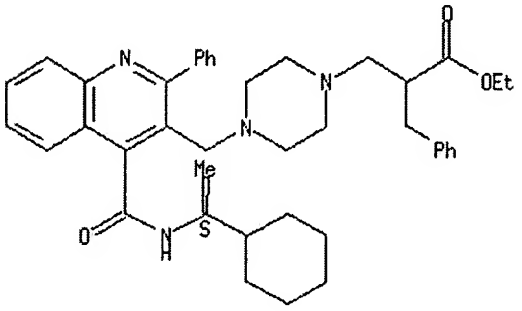
Absolute stereochemistry.



IT **433962-85-7P 433962-87-9P 433962-89-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of piperazinylalkyl quinolinecarboxamides as NK-3 and NK-2 antagonists for treatment of respiratory diseases and CNS disorders)

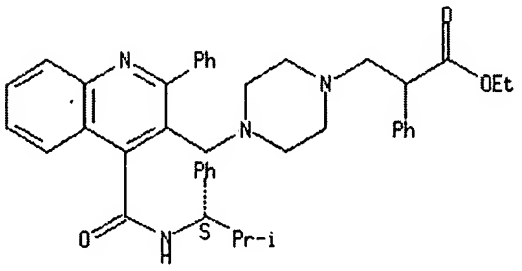
RN 433962-85-7 CAPLUS
CN 1-Piperazinepropanoic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-2-phenyl-3-quinolinyl]methyl]-α-(phenylmethyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



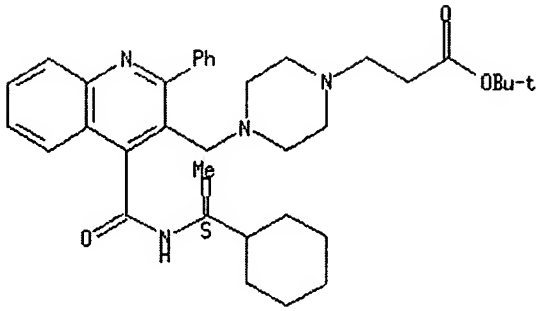
RN 433962-87-9 CAPLUS
CN 1-Piperazinepropanoic acid, 4-[[4-[[[(1S)-2-methyl-1-phenylpropyl]amino]carbonyl]-2-phenyl-3-quinolinyl]methyl]-α-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 433962-89-1 CAPLUS
CN 1-Piperazinepropanoic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-2-phenyl-3-quinolinyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
Full Text
AN 2002:368456 CAPLUS
DN 136:386030
TI Quinoline derivatives as NK-3 and NK-2 antagonists
IN Farina, Carlo; Gagliardi, Stefania; Giardina, Giuseppe; Grugni, Mario; Martinelli, Marisa; Nadler, Guy Marguerite Marie Gerard
PA Glaxosmithkline S.p.A., Italy; Laboratoire Glaxosmithkline
SO PCT Int. Appl., 71 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002038547	A1	20020516	WO 2001-EP13139	20011112
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2002020702	A5	20020521	AU 2002-20702	20011112
	EP 1334089	A1	20030813	EP 2001-993602	20011112
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2004517062	T2	20040610	JP 2002-541083	20011112
	US 2004082589	A1	20040429	US 2003-416596	20031023
PRAI	GB 2000-27696	A	20001113		
	GB 2001-9119	A	20010411		
	WO 2001-EP13139	W	20011112		

OS MARPAT 136:386030
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

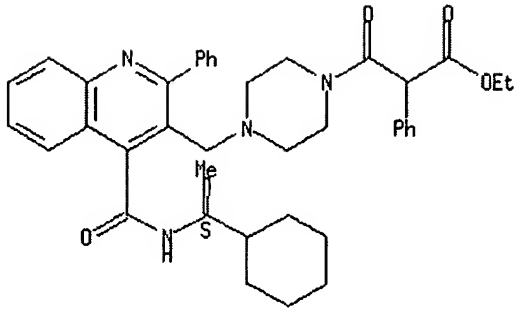
AB Title compds. I and their pharmaceutically acceptable salts or hydrates are claimed [wherein: R1 = H or alkyl; R2 = aryl, cycloalkyl, or heteroaryl; R3 = H or C1-3 alkyl, (un)substituted by 1 or more fluorines; R4 = H, R8NR9R10, R11R13, or R11R12R13; R5 = branched or linear alkyl, cycloalkyl(alkyl), aryl(alkyl), or single or fused-ring arom. heterocyclic group; R6 = H, or 1-3 of alkyl, alkenyl, aryl, alkoxy, OH, halo, NO2, cyano, CO2H, carboxamido, sulfonamido, alkoxycarbonyl, CF3, acyloxy, (di)(alkyl)amino; R7 = H, halo; n = 1-6; R8 = bond or alkylene; R9, R10 = H, alkyl, cycloalkyl(alkyl), aryl(alkyl); or NR9R10 = (un)satd. (fluoro)heterocyclyl; R11 = alkyl, alkenyl, (hetero)aryl, (un)satd. carbocyclyl with ≥1 N/O/S atom(s), cycloalkyl, etc.; R12 = (un)substituted alkyl, alkoxy; R13 = H, CO2R14; R14 = H, alkyl; any of R2, R5, R8, R9, R10, R11, R12, and R14 may be substituted by halo, OH, amino, cyano, NO2, CO2H, or oxo; with specific exclusion of 14 compds.]. Also claimed is a process for prepg. the compds., pharmaceutical compns. comprising them, and their use in medicine. I are a novel class of potent non-peptide NK-3 antagonists, some of which fall within the generic scope of WO 00/31037. I are also far more stable from a metabolic point of view than the known peptidic NK-3 receptor antagonists (no data), and are of potential therapeutic utility. I also have good NK-2 antagonist activity, and are therefore considered to be of potential use in the prevention and treatment of a wide variety of clin. conditions which are characterized by overstimulation of tachykinin receptors, in particular NK-3 and NK-2. I also show improved oral bioavailability (no data). Approx. 25 specific (S)-isomeric compds. I were prepd., and their general stereochem. forms are claimed. For instance, 3-methyl-2-phenylquinoline-4-carboxylic acid was subjected to a sequence of: (1) Me esterification; (2) α-bromination; (3) amination of the bromide with Fmoc-piperazine; (4) ester hydrolysis; (5) amidation with (S)-1-phenylpropylamine; (6) deprotection at Fmoc; (7) coupling with N-BOC-β-alanine; and (8) deprotection at BOC; to give title compd. II, isolated as the di-HCl salt. In binding assays using human and guinea pig NK-3 receptors, and human NK-2 receptors, the most potent I had IC50 values in the range of 0.1-1000 nM for NK-3, and 0.5-1000 nM for NK-2. Antagonist behavior of I at NK-3 receptors was evidenced by reversal of the effects of senktide and NKB, and antagonist activity at NK-2 receptors was indicated by reversal of the effects of NKA.

IT **425621-77-8P**, 3-[4-[[4-[((S)-1-Cyclohexylethyl)carbamoyl]-2-phenylquinolin-3-yl]methyl]piperazin-1-yl]-3-oxo-2-phenylpropionic acid ethyl ester
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; prepn. of quinoline derivs. as NK-3 and NK-2 antagonists)

RN 425621-77-8 CAPLUS

CN 1-Piperazinepropanoic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-2-phenyl-3-quinolinyl]methyl]-β-oxo-α-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

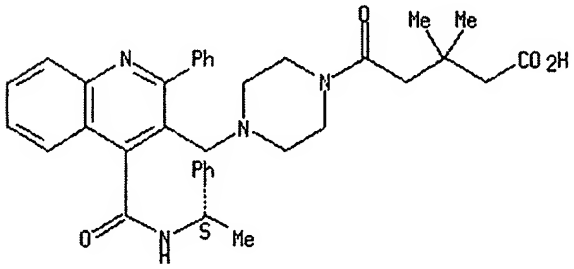
Absolute stereochemistry.



IT **425621-67-6P**, 3,3-Dimethyl-5-oxo-5-[4-[[2-phenyl-4-[((S)-1-phenylethyl)carbamoyl]quinolin-3-yl]methyl]piperazin-1-yl]pentanoic acid **425621-70-1P**, (E)-4-Oxo-4-[4-[[2-phenyl-4-[((S)-1-phenylethyl)carbamoyl]quinolin-3-yl]methyl]piperazin-1-yl]but-2-enoic acid **425621-71-2P**, 3-[4-[[4-[((S)-1-Cyclohexylethyl)carbamoyl]-2-phenylquinolin-3-yl]methyl]piperazin-1-yl]-3-oxopropionic acid **425621-72-3P**, 5-[4-[[4-[((S)-1-Cyclohexylethyl)carbamoyl]-2-phenylquinolin-3-yl]methyl]piperazin-1-yl]-5-oxopentanoic acid **425621-78-9P**, 3-[4-[[4-[((S)-1-Cyclohexylethyl)carbamoyl]-2-phenylquinolin-3-yl]methyl]piperazin-1-yl]-3-oxo-2-phenylpropionic acid sodium salt **425621-91-6P**, 3,3-Dimethyl-5-oxo-5-[4-[[2-phenyl-4-[(1-phenylethyl)carbamoyl]quinolin-3-yl]methyl]piperazin-1-yl]pentanoic acid **425621-94-9P**, 4-Oxo-4-[4-[[2-phenyl-4-[(1-phenylethyl)carbamoyl]quinolin-3-yl]methyl]piperazin-1-yl]but-2-enoic acid **425621-95-0P**, 3-[4-[[4-[(1-Cyclohexylethyl)carbamoyl]-2-phenylquinolin-3-yl]methyl]piperazin-1-yl]-3-oxopropionic acid **425621-96-1P**, 5-[4-[[4-[(1-Cyclohexylethyl)carbamoyl]-2-phenylquinolin-3-yl]methyl]piperazin-1-yl]-5-oxopentanoic acid **425622-01-1P**, 3-[4-[[4-[(1-Cyclohexylethyl)carbamoyl]-2-phenylquinolin-3-yl]methyl]piperazin-1-yl]-3-oxo-2-phenylpropionic acid ethyl ester **425622-02-2P**, 3-[4-[[4-[(1-Cyclohexylethyl)carbamoyl]-2-phenylquinolin-3-yl]methyl]piperazin-1-yl]-3-oxo-2-phenylpropionic acid
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; prepn. of quinoline derivs. as NK-3 and NK-2 antagonists)

RN 425621-67-6 CAPLUS
CN 1-Piperazinepentanoic acid, β,β-dimethyl-δ-oxo-4-[[2-phenyl-4-[[[(1S)-1-phenylethyl]amino]carbonyl]-3-quinolinyl]methyl]- (9CI) (CA INDEX NAME)

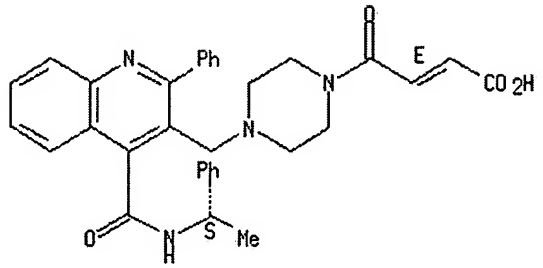
Absolute stereochemistry.



RN 425621-70-1 CAPLUS
CN 2-Butenoic acid, 4-oxo-4-[4-[[2-phenyl-4-[[[(1S)-1-

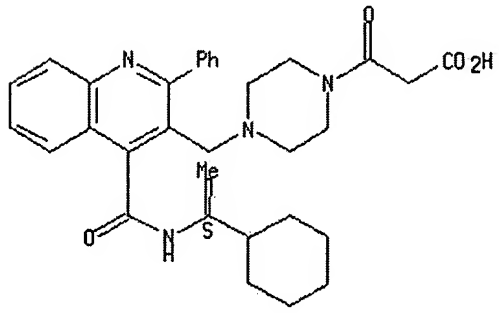
phenylethyl]amino]carbonyl]-3-quinolinyl]methyl]-1-piperazinyl]-, (2E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



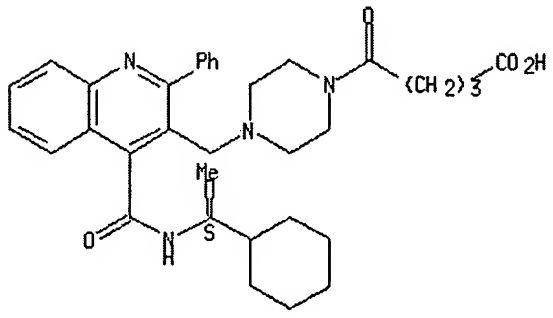
RN 425621-71-2 CAPLUS
CN 1-Piperazinepropanoic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl
]-2-phenyl-3-quinolinyl]methyl]-β-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



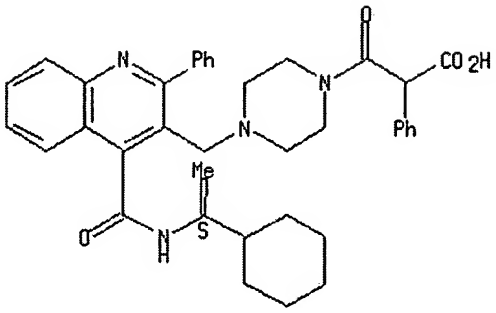
RN 425621-72-3 CAPLUS
CN 1-Piperazinepentanoic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl
]-2-phenyl-3-quinolinyl]methyl]-δ-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



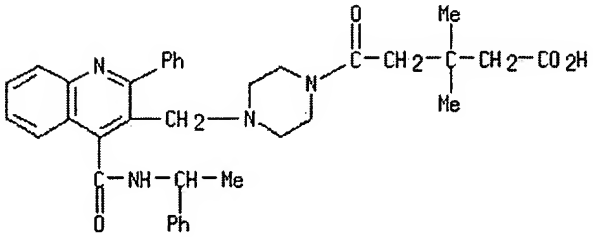
RN 425621-78-9 CAPLUS
CN 1-Piperazinepropanoic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl
]-2-phenyl-3-quinolinyl]methyl]-β-oxo-α-phenyl-, monosodium
salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

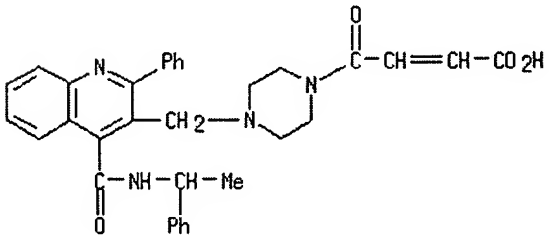


Na

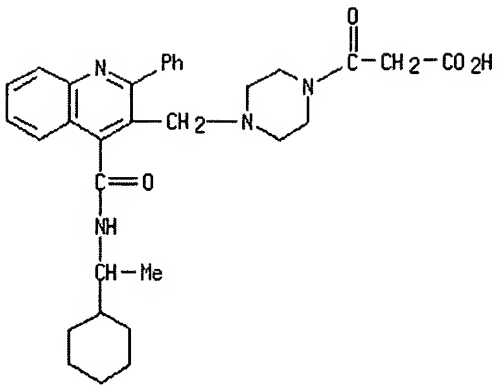
RN 425621-91-6 CAPLUS
CN 1-Piperazinepentanoic acid, β,β-dimethyl-δ-oxo-4-[[2-phenyl-4-[[(1-phenylethyl)amino]carbonyl]-3-quinolinyl]methyl]- (9CI) (CA INDEX NAME)



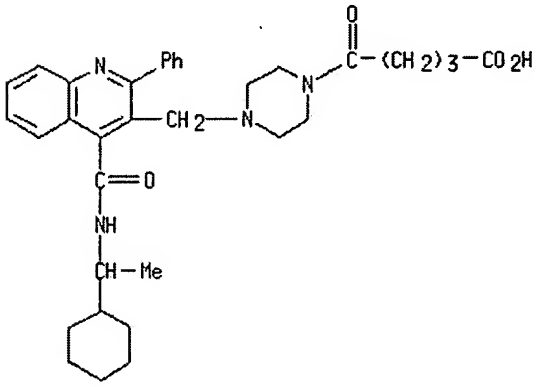
RN 425621-94-9 CAPLUS
CN 2-Butenoic acid, 4-oxo-4-[4-[[2-phenyl-4-[[(1-phenylethyl)amino]carbonyl]-3-quinolinyl]methyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)



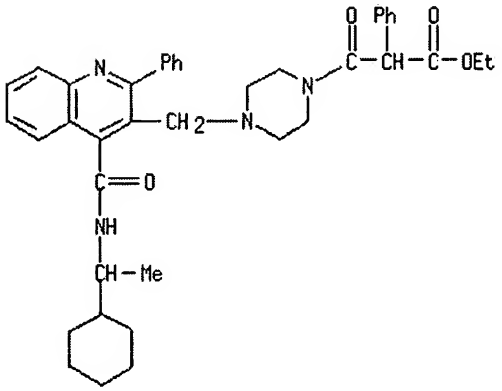
RN 425621-95-0 CAPLUS
CN 1-Piperazinepropanoic acid, 4-[[4-[[(1-cyclohexylethyl)amino]carbonyl]-2-phenyl-3-quinolinyl]methyl]-β-oxo- (9CI) (CA INDEX NAME)



RN 425621-96-1 CAPLUS
CN 1-Piperazinepentanoic acid, 4-[[4-[[(1-cyclohexylethyl)amino]carbonyl]-2-phenyl-3-quinolinyl]methyl]-δ-oxo- (9CI) (CA INDEX NAME)

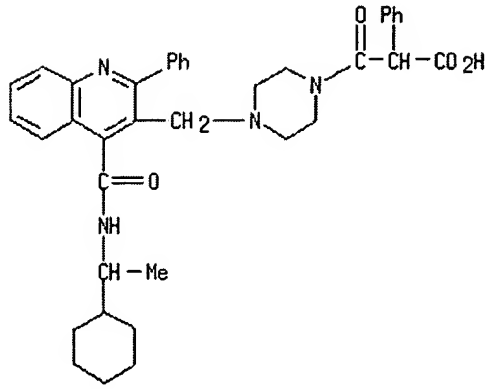


RN 425622-01-1 CAPLUS
CN 1-Piperazinepropanoic acid, 4-[[4-[[(1-cyclohexylethyl)amino]carbonyl]-2-phenyl-3-quinolinyl]methyl]-β-oxo-α-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 425622-02-2 CAPLUS
CN 1-Piperazinepropanoic acid, 4-[[4-[[(1-cyclohexylethyl)amino]carbonyl]-2-

phenyl-3-quinolinyl]methyl]-β-oxo-α-phenyl- (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
Full Text
AN 2000:368301 CAPLUS
DN 133:4605
TI Preparation of quinoline-4-carboxamide derivatives as NK-3 and NK-2 receptor antagonists
IN Farina, Carlo; Giardina, Giuseppe; Grugni, Mario; Morvan, Marcel; Nadler, Guy Margueritte Marie Gerard; Raveglia, Luca Francesco
PA Smithkline Beecham S.P.A., Italy; Smithkline Beecham Laboratoires Pharmaceutiques
SO PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000031037	A1	20000602	WO 1999-EP9115	19991119
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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BR 9915475	A	20011218	BR 1999-15475	19991119
NZ 511777	A	20031219	NZ 1999-511777	19991119
AU 768708	B2	20040108	AU 2000-17770	19991119
NO 2001002473	A	20010718	NO 2001-2473	20010518
ZA 2001004071	A	20030107	ZA 2001-4071	20010518
US 2003212101	A1	20031113	US 2003-358938	20030205

	US 6780875	B2	20040824
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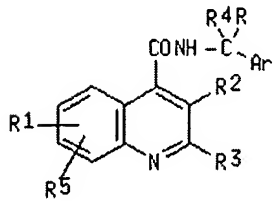
	GB 1998-25553	A	19981120
	WO 1999-EP9115	W	19991119
	US 2001-856085	B1	20010904
	US 2002-159218	B1	20020531

OS MARPAT 133:4605

GI



I

AB The title compds. of formula I [Ar = optionally substituted aryl or a C5-7 cycloalkdienyl group, or an optionally substituted C5-7 cycloalkyl group, or an optionally substituted single or fused ring arom. heterocyclic group; R = H, linear or branched C1-6 alkyl, C3-7 cycloalkyl, C3-7 cycloalkylalkyl, R1 = H or up to three optional substituents selected from the list consisting of: C1-6 alkyl, C1-6 alkenyl, aryl, C1-6 alkoxy, OH, halogen, NO2, CN, etc; R2 = (CH2)nNY1Y2; n = an integer ranging from 1 - 9; Y1, Y2 independently = (un)substituted C1-6 alkyl or together with N to which they are attached represent optionally substituted N linked single or fused ring heterocyclic group; R3 = branched or linear C1-6 alkyl, C3-7 cycloalkyl, C4-7 cycloalkyl, etc; R4 = H, C1-6 alkyl; R5 = H, halogen] useful as NK-3 and NK-2 receptor antagonists (no data given) are prepd.

IT **270573-88-1P 270573-91-6P 270573-98-3P**

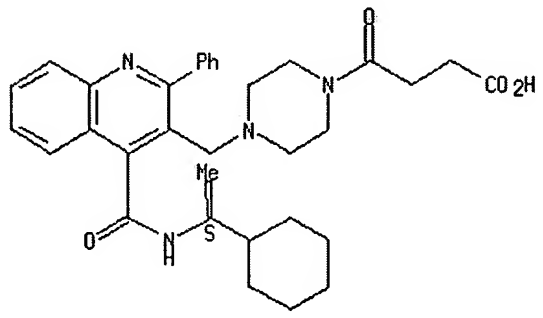
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of quinoline-4-carboxamide derivs. as NK-3 and NK-2 receptor antagonists)

RN 270573-88-1 CAPLUS

CN 1-Piperazinebutanoic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-2-phenyl-3-quinolinyl]methyl]-γ-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

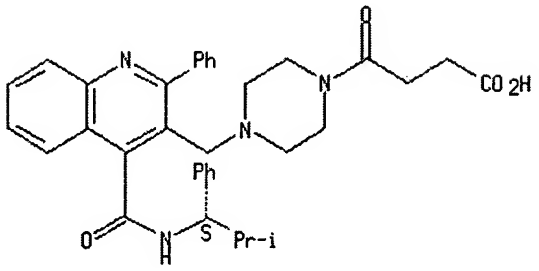


RN 270573-91-6 CAPLUS

CN 1-Piperazinebutanoic acid, 4-[[4-[[[(1S)-2-methyl-1-phenylpropyl]amino]carbonyl]-2-phenyl-3-quinolinyl]methyl]-γ-oxo-

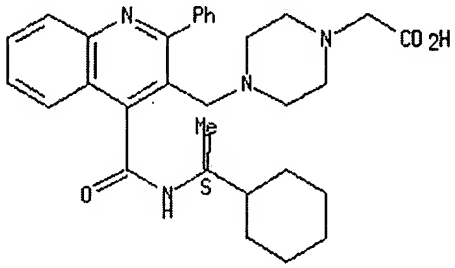
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 270573-98-3 CAPLUS
CN 1-Piperazineacetic acid, 4-[[4-[[[(1S)-1-cyclohexylethyl]amino]carbonyl]-2-phenyl-3-quinolinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.80	-2.80

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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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  This file supports REG1stRY for direct browsing and searching of
  all substance data from the REGISTRY file.  Enter HELP FIRST for
  more information.

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L5            0 L3

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